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Two Generalizations of η Pairing in Extended Hubbard Models

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The Hubbard model in bipartite lattice has been rigorously proved to have η-paired state as its eigenstates in Ref.[1]. In this paper, this result is first generalized to triangular lattice, and then even arbitrary lattice structure. Then we also consider its generalization to higher-spin Hubbard models. The conditions under which these models have η-paired states as its eigenstates were obtained.

I. INTRODUCTION

The fermionic model can possess off-diagonal long range order(ODLRO) and thus becomes superconducting via particle pairing[2]. The usual BCS state does have ODLRO via the mechanism of Cooper pairing, but it is not an eigenstate of a Hamiltonian with a local interacting term. Thus, it is of long-standing interests to find out models whose eigenstates possess ODLRO. One of the exact results about this has been obtained in Ref.[1], in which a local two-particle pairing operator called η-pairing was constructed and proved to be an eigen-operator of spin-1/2 Hubbard model in square lattice. Thus the states created by the η operator are exact eigenstates of the Hubbard model and display ODLRO.

As one of the few rigorous results about the Hubbard model in higher dimension, the η pairing has attracted a lot of theoretical interests since it was proposed. Although in the strong repulsive interaction case these eigenstates created by the η operator, which are all doubly-occupied states, have a large excitation energy, and therefore is not closely related to current discussion of high-Tc superconductivity of Cuprates in the content of $t-J$ model, the η operator has been found very helpful and widely used in the study of attractive Hubbard model[3,4,5]. Although in the majority of cases the η-pairing state is an excited state, it has been found to be ground state for some extended Hubbard models, such as in presence of nearest-neighbor interaction, bond-charge interaction and so on[6,7]. Besides, the properties of η-pairing operator have also been used to construct an $SU(2)$ symmetry group of the Hubbard model[8]. Together with another $SU(2)$ group generated by particle-hole operators, an $SO(4)$ symmetry of the Hubbard model has been found, which unifies the spin order and superconductor pairing order[9].

Recently, rapid theoretical and experimental development has been made in the field of ultracold atoms, among which the successful application of optical lattice technique is a remarkable one.[10] The fermionic atoms confined in optical lattice can be described by (extended) Hubbard models. Using the technique of quantum optics, various lattice structures can be realized[11]. It was also proposed that the tunnelling elements between nearest lattice sites can also be experimentally controlled so that the atoms in optical lattice can be effectively viewed as charged particles moving in a magnetic field[12,13]. In this paper, we will try to generalize the η-paring to the triangular lattice, and even to arbitrary lattice structures.

On the other hand, the lattice atomic gases also provide a testing grounds to study high-spin extension of Hubbard models, and the interaction between atoms is spin-dependent and can be tuned in a wide range due to the Feshbach resonance technique. Recently, Wu, Hu and Zhang discussed interacting spin-3/2 fermion atoms in optical lattice. They found that this model not only possesses a generic $SO(5)$ symmetry formed by particle-hole operators, but also has an $SU(2)$ symmetry constructed by η paring operators in the condition of some special interaction parameters.[14] We will also discuss the η-pairing for more higher spin models in the following.

We organize this report as follows. In the second section we will briefly review the keys to obtain the commutation relation $[\hat{\eta}^\dagger, \hat{H}] = C\eta^\dagger$ for spin-1/2 Hubbard model in square lattice, where $\hat{H}$ is the Hamiltonian and C is a constant. In the third section we will generalize it to Hubbard model in triangular lattice. Because the triangular lattice is not a bipartite lattice, the η operator is generally not an eigen-operator of the kinetic energy term. However, we find for a class of special hopping elements, a modified η operator can be eigen-operator. In the fourth section, we will discuss the interacting fermions with higher spins. We will answer the question that how to choose the interacting parameters so that an extended η operator can be an eigen-operator.

II. THE η PAIRING

Before discussing the generalization, we should first remind ourselves of some basic ideas of the η pairing discussed in Ref.[1] for the Hubbard model on two-dimensional square lattice, whose Hamiltonian is written as

$$\hat{H} = \hat{T} + \hat{V} = -t\sum_{ij}(a^\dagger_{\uparrow i}a_{\uparrow j} + a^\dagger_{\downarrow i}a_{\downarrow j} + h.c.) + U\sum_i n_{\uparrow i}n_{\downarrow i}. \tag{1}$$

A two-particle pairing operator of spin-1/2 fermions can be generally written as

$$\eta = \sum_{\vec{k}} g(\vec{k}) a^\dagger_{\uparrow\vec{k}} a^\dagger_{\downarrow\vec{q}-\vec{k}}, \tag{2}$$

it is an eigen-operator of the interaction energy term when $\langle n'|\hat{V}|n'\rangle - \langle n|\hat{V}|n\rangle$ is a constant for any $|n\rangle$ and

$|n'\rangle$, for which $\langle n|\eta^\dagger|n'\rangle$ is nonvanishing. Here the states $|n\rangle$ are all eigenstates of the interaction term and they form a complete bases of the Hilbert space. Noticing that the interaction terms are all local, the pairing should also be a local one, which means that $g(\vec{k})$ should be taken as a constant independent of $\vec{k}$.

In the momentum space the kinetic energy term can be written as

$$\hat{T} = \sum_{\vec{k}\sigma} f(\vec{k}) a^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} \tag{3}$$

with

$$f(\vec{k}) = -2t(\cos k_x + \cos k_y). \tag{4}$$

In Ref.[1] it is noticed that the η operator commutes with the kinetic energy term when $\vec{q}$ is taken as $\vec{\pi}$ because

$$\cos k + \cos(\pi - k) = 0. \tag{5}$$

Thus in the coordinate space the η pairing is a superposition of local particle pairs

$$\eta = \sum_{\vec{r}} e^{i\vec{\pi}\cdot\vec{r}} a^\dagger_{\uparrow\vec{r}} a^\dagger_{\downarrow\vec{r}}, \tag{6}$$

where one essential point is the sign of the pair in one site should be different from those in its nearest-neighbors. Hence the η operator thus defined satisfies the commutation relation

$$\eta^\dagger H - H\eta^\dagger = -2U\eta^\dagger. \tag{7}$$

III. GENERALIZATION TO TRIANGULAR LATTICE

We notice that the above discussion about η pairing relies on whether the lattice structure is bipartite, because the lattice structure directly determines the explicit form of $f(\vec{k})$, which plays a crucial role in finding η operator. Hence, for the Hubbard model in triangular lattice, the η paring operator introduced in previous section is not generally an eigen-operator. Then the question arouses that under which condition the model has a pairing operator as its eigen-operator.

The Hamiltonian of the Hubbard model in a triangular lattice under consideration is written as

$$\hat{H} = \sum_{ij\sigma} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{\uparrow i} n_{\downarrow i} \tag{8}$$

First focusing on the case with translational invariance, the kinetic energy term $\hat{T}$ can be written in a general form

$$\hat{T} = -t\sum_{i\sigma}\Big(e^{i\theta_1} a^\dagger_{ij,\sigma} a_{i+1j,\sigma} + e^{i\theta_2} a^\dagger_{ij,\sigma} a_{i+\frac{1}{2}j+\frac{\sqrt{3}}{2},\sigma} + e^{i\theta_3} a^\dagger_{ij} a_{i+\frac{1}{2}j-\frac{\sqrt{3}}{2},\sigma} + h.c.\Big). \tag{9}$$

Here θ_i are the phases defined in links, whereas only $\prod_{\text{closed loop}} e^{i\theta_i}$ are gauge invariant quantities, which represent the flux number through the closed loops. In the momentum space, the kinetic energy term can be written as

$$\begin{aligned}\hat{T} &= -2t\sum_{k_x k_y \sigma}\Big[\cos(k_x+\theta_1) + \cos\Big(\frac{k_x}{2} + \frac{\sqrt{3}}{2}k_y + \theta_2\Big) \\ &+ \cos\Big(\frac{k_x}{2} - \frac{\sqrt{3}}{2}k_y + \theta_3\Big)\Big] a^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} \\ &= -4t\sum_{k_x k_y \sigma}\Big[\cos\Big(\frac{k_x}{2} + \frac{\theta_1}{2} - \frac{\pi}{4}\Big)\sin\Big(\frac{\pi}{4} - \frac{\theta_1}{2} - \frac{k_x}{2}\Big) \\ &+ \cos\Big(\frac{k_x}{2} + \frac{\theta_2+\theta_3}{2}\Big)\cos\Big(\frac{\sqrt{3}}{2}k_y + \frac{\theta_2-\theta_3}{2}\Big)\Big] a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}.\end{aligned} \tag{10}$$

We notice that when $\theta_1 - \theta_2 - \theta_3 = \pi/2$, the expression of $f(\vec{k})$ turns out to be

$$\begin{aligned} f(\vec{k}) &= -4t\cos\Big(\frac{k_x}{2} + \frac{\theta_1}{2} - \frac{\pi}{4}\Big) \\ &\Big[\sin\Big(\frac{\pi}{4} - \frac{\theta_1}{2} - \frac{k_x}{2}\Big) + \cos\Big(\frac{\sqrt{3}}{2}k_y + \frac{\theta_2-\theta_3}{2}\Big)\Big],\end{aligned} \tag{11}$$

In this case, because

$$f(k_x,k_y) + f\Big(2\pi - k_x, \frac{2}{\sqrt{3}}(\theta_3-\theta_2) - k_y\Big) = 0 \tag{12}$$

the η operator defined as $\eta^\dagger = \sum_{\vec{k}} a^\dagger_{\uparrow\vec{k}} a^\dagger_{\downarrow\vec{q}-\vec{k}}$ with $\vec{q}$ taken as $(2\pi, \frac{2}{\sqrt{3}}(\theta_3-\theta_2))$ is an eigen-operator of this model.

Therefore we have succeeded in obtaining a sufficient condition for the η pairing states being eigenstates, which is $\theta_1 - \theta_2 - \theta_3 = \pi/2$. A typical configuration is plotted in Fig.1. This condition in fact means that there is a $\pi/2$ flux through each plaquette.

Furthermore, we notice that the η operator is a local operator, and the kinetic energy term only involves nearest-neighbors hopping, the assumption of translational invariance is indeed not essential. Let $t_{ij} = |t|e^{i\theta_{ij}}$, the condition can be further extended to

$$\sum_C \theta_{ij} = \frac{\pi}{2}(\text{mod}\pi), \tag{13}$$

where C stands for any closed loop with odd numbers of links. This criterion can be easily verified in the coordinate space representation, and it is valid for any other lattice structure. One can see that the bipartite lattice is just a special case of this criterion, because any closed loop in a bipartite lattice must contain even numbers of links.

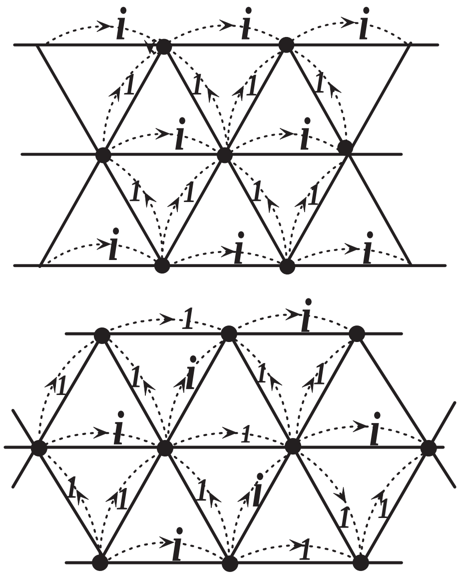

FIG. 1: Two typical configurations of hopping elements t_{ij}, which satisfy the requirement Eq.(13). The number 1 or i denotes the hopping elements t_{ij} form one site to another site. For the upper one, the Hamiltonian has translational invariance, and for the lower one it is not translational invariant.

IV. GENERALIZATION TO HIGH SPINS FERMIONS

In this section we will consider an interacting spin-$\frac{2n-1}{2}$ fermions model, with $2n$ different spin states in each site. In this model, the two-particle pairing operator is generally not eigen-operator of the interaction term because of the enlargement of the Hilbert space. It is our interest to find out an extended η operator and when the pairing operator is an eigen-operator of the interaction term $\hat{V}$.

We consider the extended Hubbard model as

$$\hat{H} = \sum_{ij\sigma} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \hat{V}, \tag{14}$$

where t_{ij} satisfy the criterion Eq.(13). It can be shown that a better choice of the on-site interaction should be like

$$\begin{aligned}\hat{V} &= V_2(a^\dagger_\uparrow a_\uparrow a^\dagger_\downarrow a_\downarrow + b^\dagger_\uparrow b_\uparrow b^\dagger_\downarrow b_\downarrow + c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow + \cdots) \\ &+V_0 \sum_{\sigma,\sigma'} (a^\dagger_\sigma a_\sigma b^\dagger_{\sigma'} b_{\sigma'} + a^\dagger_\sigma a_\sigma c^\dagger_{\sigma'} c_{\sigma'} + b^\dagger_\sigma b_\sigma c^\dagger_{\sigma'} c_{\sigma'} + \cdots) \\ &+V_1(a^\dagger_\uparrow a^\dagger_\downarrow b_\uparrow b_\downarrow + h.c. + a^\dagger_\uparrow a^\dagger_\downarrow c_\uparrow c_\downarrow + h.c. + \cdots). \end{aligned} \tag{15}$$

Here we denote $a_\uparrow$ and $a_\downarrow$ as fermionic annihilation operators for $\pm 1/2$ states, $b_\uparrow$ and $b_\downarrow$ for $\pm 3/2$ states and so on, i.e.

$$[a_\sigma, a^\dagger_{\sigma'}]_+ = \delta_{\sigma\sigma'} \tag{16}$$

and

$$[a_\sigma, b^\dagger_{\sigma'}]_+ = 0. \tag{17}$$

The first term describes the interaction between $m/2$ state and $-m/2$ state, the second describes the interaction between $\pm m/2$ states and $\pm m'/2$ states with different m and m', and the last term describes the spin flipping processes in the channel of total S_z equalling to zero. The interacting between two spin-3/2 atoms discussed in Ref.[14] is a special case of this form. One can find that the presence of the spin-flipping term is a consequence of spin-dependent interaction.

It is illuminating to consider the commutation relation between $a^\dagger_\uparrow a^\dagger_\downarrow$ and these terms. For the first term, the commutation relation is

$$[a^\dagger_\uparrow a^\dagger_\downarrow, a^\dagger_\uparrow a_\uparrow a^\dagger_\downarrow a_\downarrow]_- = -a^\dagger_\uparrow a^\dagger_\downarrow. \tag{18}$$

For the second term we have

$$[a^\dagger_\uparrow a^\dagger_\downarrow, a^\dagger_\uparrow a_\uparrow b^\dagger_\sigma b_\sigma]_- = -a^\dagger_\uparrow a^\dagger_\downarrow b^\dagger_\sigma b_\sigma, \tag{19}$$

and for the spin flipping term

$$[a^\dagger_\uparrow a^\dagger_\downarrow, b^\dagger_\uparrow b^\dagger_\downarrow a_\uparrow a_\downarrow]_- = -b^\dagger_\uparrow b^\dagger_\downarrow a^\dagger_\uparrow a_\uparrow - b^\dagger_\uparrow b^\dagger_\downarrow a^\dagger_\downarrow a_\downarrow + b^\dagger_\uparrow b^\dagger_\downarrow. \tag{20}$$

Hence, to satisfy the requirement $\eta^\dagger V - V\eta^\dagger \propto \eta^\dagger$, the terms such as $a^\dagger_\uparrow a^\dagger_\downarrow b^\dagger_\sigma b_\sigma$ should be cancelled with each other, which means that the η operator should be taken as

$$\eta = \sum_{\vec{r}} e^{i\vec{q}\vec{r}} (a^\dagger_{\vec{r}\uparrow} a^\dagger_{\vec{r}\downarrow} + b^\dagger_{\vec{r}\uparrow} b^\dagger_{\vec{r}\downarrow} + c^\dagger_{\vec{r}\uparrow} c^\dagger_{\vec{r}\downarrow} + \cdots), \tag{21}$$

and the parameters in Eq.(15) should satisfy the requirement

$$V_1 = -2V_0. \tag{22}$$

This relation recovers the result obtained in Ref.[14]. The commutation relation is therefore

$$[\eta^\dagger, V] = -(V_2 + 2V_0)\eta^\dagger, \tag{23}$$

The generalized η-operator is also a superposition of local spin-singlet two-particle pairing. The state created by the operator has ODLRO for the same reason discussed in Ref.[1]and Ref.[2]

V. CONCLUSION AND DISCUSSION

In summary, we have discussed two generalizations of the η-paring to two kinds of extended Hubbard models. The original conclusions about the η-pairing was restricted for bipartite lattice structure, in this paper we showed that for the Hubbard model defined on any lattice structure, a modified η-operator can be the eigen-operator if the hopping elements satisfying the criterion

Eq.(13). We also discussed the η-pairing for higher-spin Hubbard models. We find that in order that the model has modified η-paired states as its eigenstates, the interaction part should contain spin-flipping term and the parameters should satisfy the condition Eq.(22).

As the original η-paired state[1], the generalized η-paired states are also usually excited states. One thing of much concern is when these generalized η-paired states become ground states. In the original paper[1], it is shown the η-paired state is metastable for attractive interaction. And later, various extended models which have the η-paired state as their ground states were proposed[6,7]. Following these ideas, how to obtain models having the generalized η-paired states as the ground states is under further consideration. We hope that these efforts could shed light on the study of fermionic atoms in optical lattice and some solid-state materials such as $NaCoO$ which have triangular lattice structure[15].

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